

MPA Materials Matter

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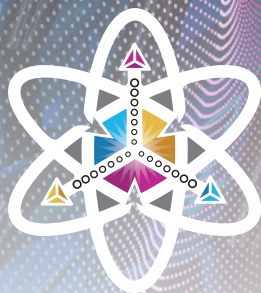
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Rod Borup

Recognized for enduring technological contributions

Rod Borup (Materials Synthesis and Integrated Devices, MPA-11) has been named a 2020 Electrochemical Society (ECS) Fellow. The distinction recognizes advanced individual technological contributions in electrochemical and solid-state science and technology and service to the society.



“Being selected as an Electrochemical Society Fellow is such a prestigious honor; this is the primary scientific community and group for us to present our fuel cell-related work, so it is great to be recognized by our scientific peers,” Borup said. “The members of ECS also represent my primary networking group where we form our collaborations, which is incredibly important for forming teams to respond to open proposals.”

Dedicated to overcoming barriers—Borup is the LANL program manager for Fuel Cells and Vehicle Technologies and the MPA-11 Fuels Cells team leader. As director of the Fuel Cell Consortium for Performance and Durability, he leads a multidisciplinary team from five national laboratories dedicated to demonstrating world-class improvements in fuel cell performance and durability, exceeding the 2020 targets set by the DOE Fuel Cell Technologies Office. He is also a research professor in the department of chemical and biological engineering at the University of New Mexico.

The cost and durability of current polymer electrolyte membrane fuel cells (PEMFCs) are major barriers to their commercial use for stationary or transportation power generation. Borup's research focuses on PEMFCs, including fuel cell component durability, water transport, electrode design, and gas-diffusion-layer materials. His work is funded primarily through the DOE Hydrogen and Fuel Cell Technologies Office.

Patents, papers, awards—Borup holds 13 U.S. patents. He has authored more than 150 papers related to fuel cell technology, garnering more than 10,000 citations and an h-index of 39. Borup, who received his doctorate in chemical engineering from the University of Washington, joined the Lab in 1994 as a postdoctoral researcher.

His recognitions include a 2016 DOE Fuel Cell Technologies Office Annual Merit Award for Fuel Cells, a 2014 Research Award of the Energy Technology Division of the Electrochemical Society, a U.S. Drive 2012 Tech Team Award for the Fuel Cell Technical Team, and a 2005 DOE Hydrogen Program R&D Award.

About ECS—Founded in 1902, ECS is the world's largest professional society for electrochemical science and applications. Its mission is to advance theory and practice at the forefront of electrochemical and solid state science and technology, and allied subjects. No more than 15 scientists and engineers are chosen annually by their peers to receive the rank of fellow.

Technical contact: Rod Borup ■



“ My philosophy is that managers should champion the scientific and programmatic goals of their organization, solve problems that are hampering the staff, and support individuals and teams to complete their projects and advance their careers.

From Wolfgang's desk ...

As your new acting deputy division leader I'd like to introduce myself. While I'm new to MPA Division, I know many of you from collaborations during my 25 years at LANL or from outside activities—like my kids' schools and activities and my main hobby, playing and coaching soccer.

I began at LANL as a postdoc, and my career has been split between Chemistry Division and LANL's Office of Science Programs. I had the opportunity to work at different levels of scientific leadership and management, from research lead to principal investigator and manager of multidisciplinary programs, and from team leader and RLM for the hot cell and the actinide research facilities at TA-48, to associate director in the National Isotope Development Center, managed by the Office of Nuclear Physics. My primary scientific area has been researching the chemical behavior of the actinide elements with applications in separations, environmental management, and national security. I am most proud of leading the effort to create the actinide research facility at TA-48 and helping advance the careers of about 30 young professionals that I recruited and mentored. For the last 12 years, I coordinated isotope production across the DOE complex, distributing critically needed radionuclides worldwide for research and commercial (medical) applications. This required continuous planning, integrating competing interests of national labs to a common goal, identifying opportunities, and adjusting to production fluctuations and changing customer needs.

My philosophy is that managers should champion the scientific and programmatic goals of their organization, solve problems that are hampering the staff, and support individuals and teams to complete their projects and advance their careers. In my various roles, I have been privileged to interact with so many people at vastly different organizations, from students to senior managers at national laboratories and DOE headquarters, university professors, leaders of international scientific organizations, and CEOs of industrial organizations. I also have gained extensive experience in program development and management, including leading three LDRD-DR teams. Having worked in and managed activities in radiologically controlled and synthetic laboratory spaces, I understand our problems in working in crowded spaces and aged facilities and operational requirements. I have a lot of experience that we can draw upon to help you accomplish your goals.

We are beginning the last quarter of the fiscal year. I realize we are all anxious about our work goals and programmatic commitments. I look forward to supporting you as we ramp back up. If you are facing challenges, please feel free to contact me at any time.

Acting MPA Deputy Division Leader Wolfgang Runde ■



“My philosophy is that underneath every applied problem is a basic science question waiting to be asked, and answered. My vision is for CINT to be the place where these questions can be asked and answered with expert assistance and state-of-the-art tools.

From Adam's desk . . .

My transition to LANL after 19 years at Oak Ridge National Laboratory has been invigorating and exciting. I loved working at Oak Ridge, but science is a creative enterprise and occasional change is necessary to stay creatively engaged.

In my new role as co-director for the Center for Integrated Nanotechnologies (CINT) and the group leader for MPA-CINT, I am responsible for defining and executing a vision for a publicly accessible user facility. When I think about a vision for CINT, I often go back to the fundamental driver for CINT's existence. We are all familiar with LANL's story originating in World War II, where scientific research led to a major advance in weapons technology and the escalation of the United States to a world power. We may not be familiar with a similar story that also began with the Manhattan Project; toward the end of WWII, President Roosevelt asked Vannevar Bush, the director of the Office of Scientific Research and Development, to investigate whether federally sponsored research could also have the same effect on *economic competitiveness* and *healthcare* as it did on military competitiveness. Bush produced a report titled *Science, the Endless Frontier*, in which he argued that scientific research is the pacemaker of technological progress. It is still well worth a read for anybody interested in publicly sponsored science.

The Bush report led directly to the establishment of the National Science Foundation in 1950 and set federal science policy on a trajectory that has not changed to this day. Since that time federal support for the physical and healthcare sciences has continued uninterrupted, although with some ups and downs, and has resulted in the development of an amazing set of technologies that contribute to our modern quality of life. The Bush report was correct in its assertion that publicly sponsored basic science leads to improved economic outcomes.

My philosophy is that underneath every applied problem is a basic science question waiting to be asked, and answered. My vision is for CINT to be the place where these questions can be asked and answered with expert assistance and state-of-the-art tools. In my perspective, a user facility like CINT serves the public in unique and important ways: it provides capability and expertise on short notice; it provides capability that is not easily duplicated or is cost prohibitive to own; it acts as a place to test novel ideas and concepts. Researchers should feel free to bring whatever problems they face to a user facility like CINT— that is our role.

CINT is a nanoscience center, but nanoscience isn't really about nanobots like we see in the popular press. It's about advanced materials, the interface of biology with materials science, new optical and electronic devices, and lately, quantum information sciences. It's also about developing new techniques to examine and understand the world around us. My goal is for CINT to be deeply integrated into the LANL mission in addition to being a national resource.

Thanks for taking the time to read this. I look forward to working with the LANL community to help make CINT and LANL successful.

Center for Integrated Nanotechnologies Co-director Adam Rondinone ■

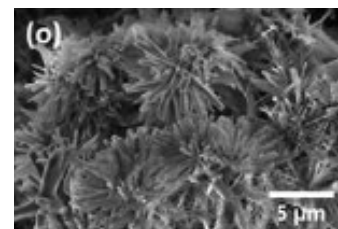
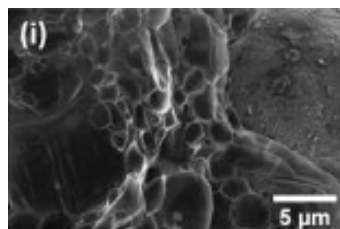
Frustrating harmful dendrite formation in potassium ion batteries

Technology addresses key factor in premature battery failure

With the rapid development of large-scale energy storage systems, “beyond lithium ion battery” chemistries are attracting extensive attention, including alternative metal ions such as potassium and sodium. Potassium batteries have the potential to deliver a low-cost, complementary technology to lithium ion batteries to the general consumer and surpass sodium, graphite, and other forms of ion batteries.

Potassium offers unique electrochemical advantages such as the highest ion mobility, conductivity, and transport number in a carbonate electrolyte. However, potassium metal anodes in battery applications can still suffer from the challenging problem of dendrite growth—a key factor in premature battery failure. Dendrites are tiny, rigid, tree-like structures that can grow inside the battery upon cycling and can cause tremendous harm.

Center for Integrated Nanotechnologies (CINT) users have developed a novel 3D electrode technology that overcomes this drawback. In research published in *Advanced Materials* they demonstrated a tailored current collector that is functionalized to create a *potassiphilic* surface. This potassium-attracting surface promotes 2D layer-by-layer growth and geometrically frustrates 3D dendrite growth. Their unique electrode contains specially coated cells that achieve state-of-the-art plating and stripping performance.



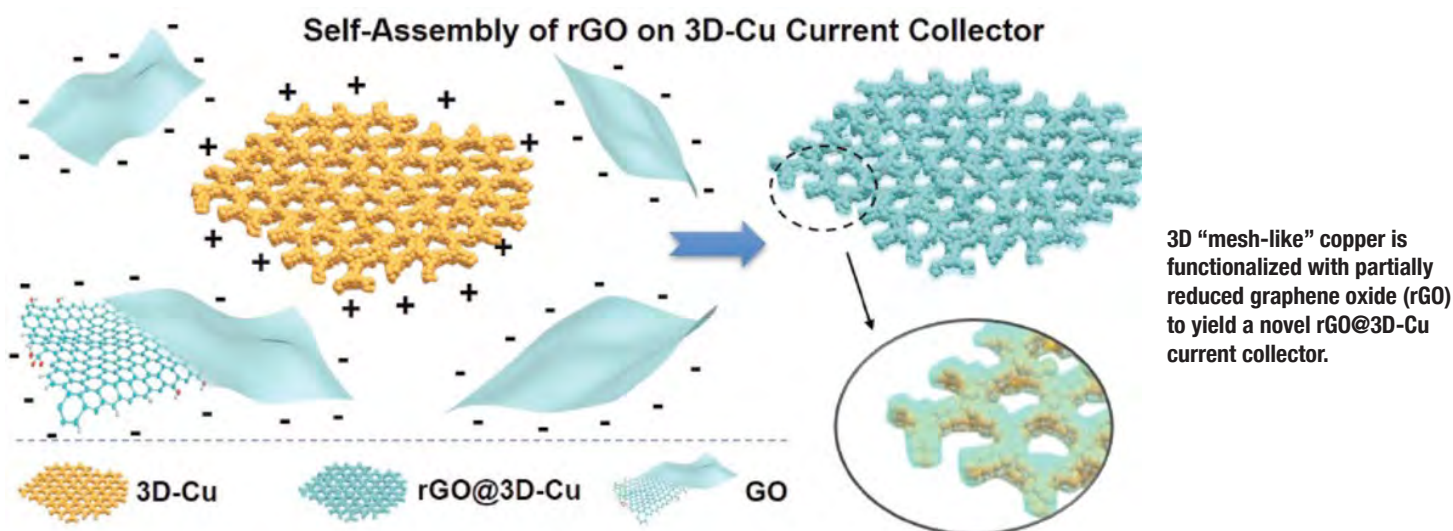
Scanning electron microscopy images showing (left) the novel rGO@3D-Cu electrode surface after 100 cycles, with no evidence of dendrite formation. Whereas a standard planar Cu surface (right) showed significant dendrite formation after only 20 cycles.

The accomplishment was supported by CINT’s unique materials characterization capabilities. CINT recently established a new cryogenic electron microscopy suite, specifically for the imaging of such low-Z and beam-sensitive materials.

The work, which supports the Lab’s Energy Security mission and its Materials for the Future science pillar, was performed in part at CINT, a DOE Office of Science Basic Energy Sciences user facility jointly operated by Sandia National Laboratories and Los Alamos National Laboratory. The Los Alamos portion of the work was funded by the DOE Office of Science, Basic Energy Sciences.

Researchers: John Watt (Center for Integrated Nanotechnologies, MPA-CINT); Pengcheng Liu, Yixian Wang, and David Mitlin (University of Texas at Austin); Qilin Gu (University of Singapore); Jagjit Nanda (Oak Ridge National Laboratory). Reference: “Dendrite-free potassium metal anodes in a carbonate electrolyte,” *Advanced Materials*, 32 (2020).

Technical contact: John Watt ■



From a Mott insulator to an ideal two-dimensional metal

In high temperature superconductivity, the pseudogap refers to a state of matter extending up to room temperature and beyond when layered copper oxides are doped with sufficient holes to transform a Mott insulator into a metal but insufficient holes to achieve optimal superconductivity.

Since it spans both the Mott insulating and superconducting regimes, the pseudogap is believed to hold the key to understanding the origin of high- T_c pairing. However, considerable debate continues as to whether or not the pseudogap constitutes a novel form of order and how exactly the gap manifests itself over the Fermi surface.

Recently, a team of researchers, including scientists from the National High Magnetic Field Laboratory-Pulsed Field Facility (MPA-MAGLAB), have performed magnetic quantum oscillation experiments on arguably the highest quality single crystals of the high- T_c superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (or YBCO for short) produced thus far and have made the surprising discovery that the material behaves much like an ideal two-dimensional metal.

Their work was published in the journal *Nature Physics*.

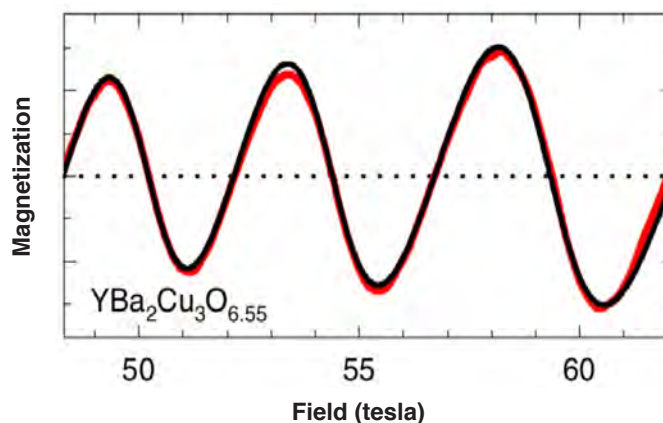
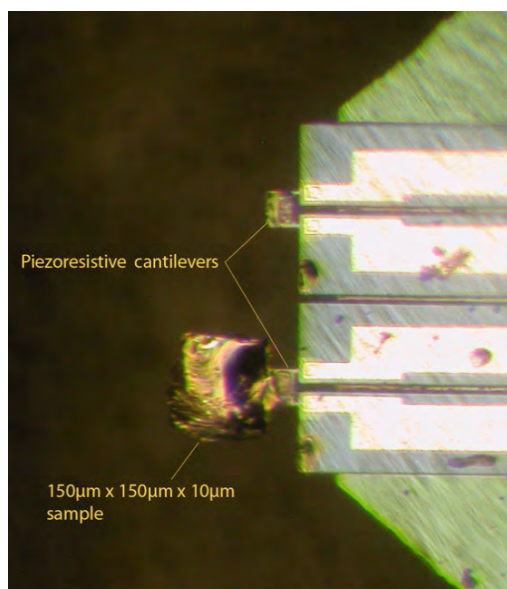
Ideal two-dimensional metals have been known to exist in GaAs heterostructures for many years but have recently also been shown to occur in graphene and on the surface of topological insulators. What the quantum oscillation experiments show is that like GaAs, the Fermi surface consists of a single pocket of carriers that exists in complete thermodynamic isolation—it behaves as if the number of particles is rigidly fixed, causing the wave form of the de Haas-van Alphen magnetic oscillations to acquire a distinctive “saw-

tooth” wave form. Since no carriers are exchanged with the surroundings, the experiments imply that the pseudogap is what can be referred to as a hard gap. Thus, with the exception of the isolated pocket of carriers, the system is completely gapped very much like it continues to be an insulator. The result matters because it significantly constrains possible origins for the pseudogap in high- T_c materials. One class of theories predicting the pseudogap to be heavily broadened by strong electronic correlations can essentially be eliminated. Rather, the existence of a hard gap with little or absent broadening points to a novel form of quantum or topological order within the pseudogap state.

The quantum oscillations were detected in the magnetic torque using a piezoelectric cantilever at the mag lab in strong magnetic fields extending to 65 tesla by a team of scientists including Neil Harrison, Mun Chan, Ross McDonald, and Kimberly Modic. The high-quality crystals were grown at the Max Planck Institute for Solid State Research in Germany and sample preparation was conducted at the Cavendish Laboratory in the United Kingdom. Additional supporting experiments were performed at the High Magnetic Field Laboratory in China. The research was funded by the Basic Energy Sciences (DOE Office of Science) “Science of 100 tesla” program and supports the Laboratory’s Energy security mission and Materials for the Future science pillar.

Reference: “Hard antinodal gap revealed by quantum oscillations in the pseudogap regime of underdoped high- T_c superconductors,” *Nature Physics*, 4 (2020).

Technical contact: Neil Harrison ■



At left, an image of a sample on a piezoresistive cantilever and (above) an example of the distinctive “sawtooth” de Haas-van Alphen oscillations in a high- T_c superconductor.

First-ever actinide-zirconium framework synthesized

Work relevant to storage and environmental fate of nuclear waste

Accurately characterizing actinide species bound to metal-organic frameworks (MOFs) is important for understanding these structures as potential radioactive waste forms and providing new models of actinide species transport in the environment. MOFs are highly tunable, porous, crystalline solids with extended structures that self-assemble from inorganic nodes and organic linkers.

Zirconium-based MOFs (Zr-MOFs) exhibit a diversity of topologies along with high chemical and thermal stability and are often accessible by scalable and green syntheses. Due to the stability of MOFs and their ability to uptake high concentrations of contaminants, they are potential nuclear waste forms. Additionally, the interaction of the uranyl species with the Zr oxide cluster provides a model for mineral absorption and transport that is easier to characterize than similar species absorbed to surfaces.

In work appearing in *Crystal Engineering Communications*, Los Alamos researchers and their external colleagues used solvothermal deposition to synthesize a uranyl-grafted framework, thus creating a single-crystal structure that is the first reported actinide ion bound in the channel of a Zr-MOF.

Hierarchical Zr-MOF was prepared in collaboration between scientists in Materials Synthesis and Integrated Devices (MPA-11) and Northwestern University. This MOF was post-synthetically modified to introduce uranyl ion into the Zr-oxide cluster unit of the MOF.

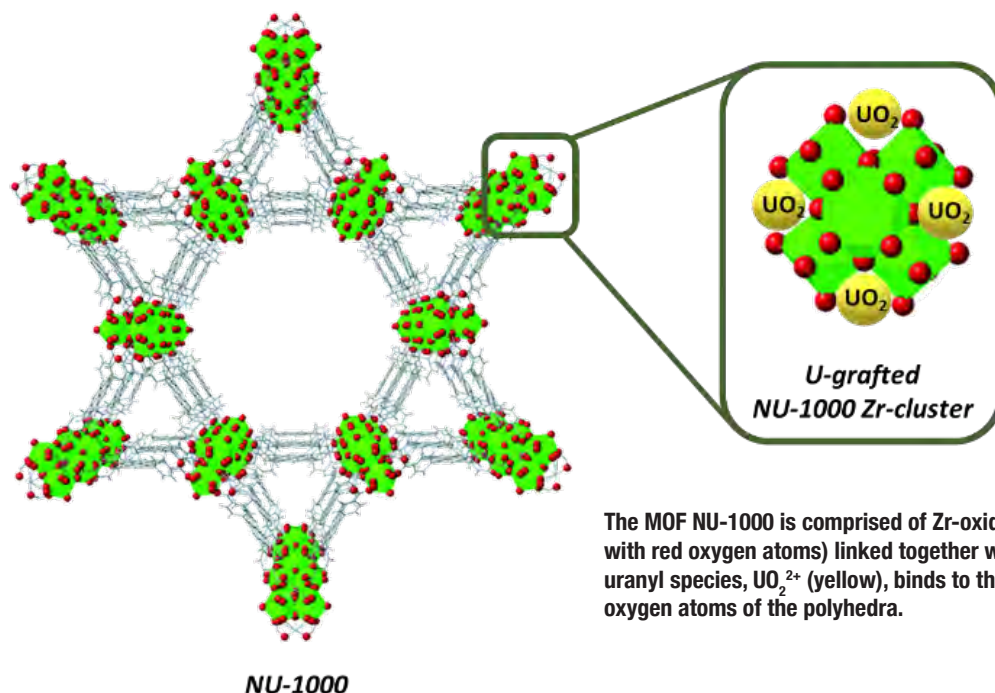
Analysis of the chemical composition of the crystals by SEM and Raman spectroscopy at LANL revealed that uranyl atom is dispersed uniformly throughout the crystal and incorporates into the framework through binding of the Zr-oxide cluster rather than metal exchange. These findings were further corroborated through determination of the single-crystal x-ray diffraction pattern for the UO_2 -Zr-MOF.

The work supports the Laboratory's Energy Security mission and its Materials for the Future science pillar. The Los Alamos portion of the work was funded by the Laboratory Directed Research and Development program.

Researchers: Tatyana Elkin, Brian L. Scott (MPA-11); Laura E. Wolfsberg (Inorganic, Isotope, and Actinide Chemistry, C-IIAC); and Julia G. Knapp, Xuan Zhang, Sylvia L. Hanna, Florencia A. Son, and Omar K. Farha (Northwestern University).

Reference: "Single crystal structure and photocatalytic behavior of grafted uranyl on the Zr-node of a pyrene-based metal-organic framework," *CrystEngComm*, 22 (2020).

Technical contact: Brian Scott ■



The MOF NU-1000 is comprised of Zr-oxide clusters (green polyhedrons with red oxygen atoms) linked together with organic linkers (gray). The uranyl species, UO_2^{2+} (yellow), binds to the Zr-oxide polyhedra through the oxygen atoms of the polyhedra.

HeadsUP!

Mechanical material handling explained

Mechanical material handling (MMH) activities happen on a regular basis, whether it is moving a multimillion-dollar piece of unique equipment or moving something as common as office furniture.

P101-40, Mechanical Material Handling, is a new policy on how to conduct safe movements of loads and reduce worker injury. The policy covers work activities involving moving materials by various types of equipment that provide a mechanical advantage.

Examples of MMH activities include

- moving materials using a cart;
- transporting gas bottles, dewars, and/or liquid cylinders using a cart or dolly;
- using hand trucks, hydraulic lift tables, and pallet jacks; and
- moving unique configurations that require the involvement of a MMH coordinator.

P101-40 fills a significant gap within LANL safety and health policies as no institutional program specific to mechanical material handling has existed. As illustrated below, MMH fits squarely between manual material handling, forklifts, and hoisting and rigging.

P101-40 includes answers for important questions, such as:

- What is the difference between an ordinary vs. critical load activity? How do you determine the difference between the two?
- How and when should MMH equipment be inspected?
- What training is required for mechanical material handling?
- What hazards need to be considered prior to moving equipment safely?
- What are the safe work practices for common types of MMH equipment such as wheeled equipment, manual pallet jacks, and drum handling/lifting equipment?
- What are the safe work practices for handling and transporting materials such as palletized drums and compressed gas cylinders?

P101-40 was provisionally issued on July 22 and will become effective on January 22, 2021. For more information on MMH, please visit the Mechanical Material Handling website.

Mechanical Material Handling program lead:
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To submit news items or for more information, contact Karen Kippen, ALDPS Communications, at 505-606-1822 or aldps-comm@lanl.gov.

For past issues, see www.lanl.gov/org/ddste/aldps/materials-physics-applications/materials-matter-archive.php.



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Celebrating service

Congratulations to the following MPA Division employees recently celebrating service anniversaries:

Scott Crooker, MPA-MAGLAB	25 years
Neil Harrison, MPA-MAGLAB.....	20 years
Roger Lujan, MPA-11	20 years
Tommy Rockward, MPA-11	20 years
Houtong Chen, MPA-CINT	15 years
Priscila Ferrari Silveira Rosa, MPA-Q	5 years
Laurel Stritzinger, MPA-MAGLAB.....	5 years